DOCUMENTATION

BIOACCUMULATION MODEL

QEAFDCHN v.1.0

Quantitative Environmental Analysis, LLC.
305 West Grand Avenue
Montvale, NJ 07645

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SECTION 1
INTRODUCTION

This document describes the model QEAFDCHN version 1.0, a modified version of FDCHN version 4.1, a program written by Dr. John Connolly while at Manhattan College. Modifications were performed at Quantitative Environmental Analysis, LLC (QEA). The computer simulation model QEAFDCHN v1.0 computes the concentrations of chemicals in aquatic biota. The framework is written in FORTRAN, compiled using DIGITAL Visual Fortran v.6.0, and is run on a Hewlett Packard Kayak (Intel Pentium II) using Windows NT. This document provides descriptions of:

- Section 2: Model structure: the number and identity of the FORTRAN files.
- Section 3: Species indexing: the way in which individual species and age classes within species are indexed in the model code
- Section 4: Input file: each parameter and line in the input file is described.
- Section 5: Output files: each entry in each output file is described.

SECTION 2
MODEL STRUCTURE

The bioaccumulation model is comprised of eight program subroutines. Each subroutine either reads or writes data or performs calculations describing specific components of the food web. An additional fortran file ("fdchn4.cmn") contains parameterization information. A brief description of each file/subroutine is detailed below.

fcmain.f

- This is the main program file. This file calls subroutines in the other files, as well as writes all model results to the output files "fdchain.out."

fcinput.f

- This file reads input information from file "fdchain.inp." It consists of one subroutine. Subroutine FCINPT reads the user-supplied input file and echoes input to the file "fdchain.out."

fcexpose.f

- This file consists of one subroutine that reads exposure information from the file "fdchain.inp." Subroutine FCEXPOSE reads the user-specified water column and sediment (dissolved and particulate) exposure concentrations for all chemicals in each compartment. It echoes this information to the file "fdchain.out."

fcfdchn.f

- This file contains the main subroutine (FDCHN) in the model that computes the transfer of contaminants through the food web. This subroutine calls the four other subroutines presented below.

fcbioeng1.f

- This file consists of subroutine BIOENG1. This subroutine calculates the bioenergetic parameters (e.g., weight, growth rate and fraction lipid) for each age-dependent species.

fcbioeng2.f

- This file consists of one subroutine (BIOENG2). Subroutine BIOENG2 calculates the respiration and ingestion rates for each age-dependent species in each spatial compartment.

fcknetic.f

- This file consists of subroutine KNETIC. Subroutine KNETIC computes the uptake rates from water and the excretion rates for all steady-state and age-dependent species.

fcssconc.f

- This file consists of one subroutine (SSCONC). Subroutine SSCONC calculates the contaminant concentrations of the steady-state species.

SECTION 3
SPECIES INDEXING

In the food web model species are indexed in two ways. Each species above the plankton-detritus level is numbered sequentially in the order in which they are listed in the input file "fdchain.inp." The steady-state species must be listed before the age-dependent species in the input file. In addition, each steady-state species and each age class of each age-dependent species is assigned a "step number", which is also specified according to the order of species in the input file.

For example, if a food web consists of plankton, a steady-state invertebrate, an age- dependent forage fish with two age classes, and an age-dependent predator fish with three age classes the steps are as follows:

		SPECIES NUMBER	STEP NUMBER
Invertebrate		1	1
Forage Fish	age 1	2	2
Forage Fish	age 2	2	3
Predator Fish	age 1	3	4
Predator Fish	age 2	3	5
Predator Fish	age 3	3	6

Thus, the species number and step number for the first age class of the predator fish are 3 and 4, respectively.

SECTION 4
INPUT FILE

Input for the bioaccumulation model includes information about the chemicals, species and compartmentalization of the study area being modeled. Input is divided into nine groups (Groups A through I), each describing a separate component of the food web. The inclusion of all input groups is not required for a successful model run. Entire groups or portions of these groups may be omitted, depending on the composition of the food web.

Two files are required to perform a food web model calculation; an input file and an executable file. The input file should be structured as an ASCII text file and have the name "fdchain.inp." The program executable file is named "qeafdchn1.exe."

The maximum values for the number of time breaks for input parameters, number of chemicals, number of migrating species, number of species, number of "steps" (i.e., the sum of all steady-state species plus all age classes in all age-dependent species), number of prey for any age class and number of spatial compartments are specified in the file "fdchn4.cmn." These values can be changed, after which all files must be recompiled and a new executable file created.

Each parameter required in the file "fdchain.inp" is described below.

GROUP A – NUMBER OF SPECIES AND CHEMICALS BEING MODELED

A1. Number of Species and Chemicals

NSP, NSPSS, NCHEM
(3I5)

NSP - number of species for which age-specific concentrations are calculated

NSPSS - number of species for which steady-state concentrations are calculated

NCHEM - number of chemicals being modeled

A2. Chemical Identification

CHEM(1), CHEM(2), CHEM(NCHEM)

(5A15)

CHEM - name of chemicals being modeled

GROUP B – CHEMICAL-SPECIFIC PARAMETERS

B1. Chemical Characteristics

KOWFLG(I), PRATIO(I), CR(I)

(I5,2F10.0)

KOWFLG(I) - flag indicating whether the BCF value is used in calculating the rate at which chemical I is eliminated

When IFLG1(I) = 1: The BCF values provided in "fdchain.inp" are used to calculate the chemical elimination rate. KOWFLG(I) is not used in the model.

When IFLG1(I) = 0 and KOWFLG(I) = 0:

BCF values provided in "fdchain.inp" are used to calculate the chemical elimination rate.

When IFLG1(I) = 0 and KOWFLG(I) = 1:

BCF values provided in "fdchain.inp" are not used in the model.

PRATIO(I) - ratio of the efficiency of contaminant transfer across the gill to the efficiency of oxygen transfer across the gill for chemical I

CR(I) - resistance factor for transfer of chemical I from lipid to blood

Group B is repeated NCHEM times; once for each chemical.

GROUP C – ENERGY RELATED PARAMETERS

C1. Phytoplankton and Sediment Parameters

PENERGY, SENERGY

(2F10.0)

PENERGY - energy density of water column particulate matter (kJ/g C)

SENERGY - energy density of sediment (kJ/g C)

GROUP D – STEADY-STATE SPECIES PARAMETERS

D1. Species Identification

IFLG(I), IFLG1(I), TITLE(I)

(2I5,A15)

IFLG(I) - flag indicating the source of the water with which the organism is in contact

IFLG(I) = 0: species (I) is in contact with the water column

IFLG(I) = 1: species (I) is in contact with benthic pore water

IFLG1(I) - flag indicating the method by which the chemical elimination rate for species I will be computed

IFLG1(I) = 0: elimination rate is proportional to the chemical uptake rate from water

When KOWFLG(I) = 0: elimination rate equals uptake rate uptake rate from water ÷ BCF

When KOWFLG(I) = 1: elimination rate equals uptake rate uptake rate from water * fraction aqueous * multiplier (C_R)

IFLG1(I) = 1: elimination rate is equal to the BCF value

TITLE(I) - name of steady-state species

D2. Bioenergetic Parameters

RESP(I), GROW(I), ASIM(I), FPROT(I), RHO(I), FLIPID(I)

(6F10.0)

RESP(I) - respiration rate of species I (kJ/g wet-day)

GROW(I) - growth rate of species I (day^{-1})

ASIM(I) - food assimilation efficiency of species I

FPROT(I) - fraction protein of species I (g protein/g wet)

RHO(I) - exponential coefficient for temperature dependence of species I respiration ($^oC^{-1}$)

FLIPID(I) - fraction of wet weight that is lipid (g lipid/g wet)

ASM(I,1), BCF(I,1) … ASM(1,NCHEM), BCF(I,NCHEM)

(8F10.0)

ASM - toxicant assimilation efficiency of species I

BCF - factor used to calculate elimination rate as specified in Group D1

LKOW - partition coefficient of chemical J in species I (L/kg)

Group D is repeated NSPSS times; once for each steady-state species.

GROUP E – AGE-DEPENDENT SPECIES PARAMETERS

E1. Species Identification

IFLG(I), IFLG1(I), TITLE(I)

(2A5,A15)

IFLG(I) - flag indicating the source of the water with which the organism is in contact

IFLG(I) = 0: species (I) is in contact with the water column.

IFLG(I) = 1: species (I) is in contact with benthic pore water

IFLG1(I) - flag indicating the method by which the chemical elimination rate for species I will be computed

IFLG1(I) = 0: elimination rate is proportional to the chemical uptake rate from water

When KOWFLG(I) = 0: elimination rate equals uptake rate uptake rate from water ÷ BCF

When KOWFLG(I) = 1: elimination rate equals uptake rate uptake rate from water * fraction aqueous * multiplier (C_R)

IFLG1(I) = 1: elimination rate is equal to the BCF value

TITLE(I) - name of age-dependent species

E2. Bioenergetic Parameters

NAC(I), ACS(I), BETA(I), GAMMA(I), ASIM(I), FPROT(I), SDA(I)

(I5, 7F10.0)

NAC(I)	- number of age classes for species I
ACS(I)	- age class size of species I (days)
BETA(I)	- respiration coefficient for species I (kJ/g wet-day)
GAMMA(I)	- respiration weight exponent for species I
ASIM(I)	- food assimilation efficiency of species I
FPROT(I)	- fraction protein of species I (g protein/g wet)
SDA(I)	- specific dynamic action of species I

RHO(I), OMGA(I), DLTA(I), PHI(I), XNU(I)

(5F10.0)

RHO(I)	- exponential coefficient for temperature dependence of species I respiration ($^oC^{-1}$)
OMGA(I)	- swimming speed coefficient for species I (cm/s)
DLTA(I)	- swimming speed weight exponent for species I
PHI(I)	- exponential coefficient for temperature dependence of species I swimming speed ($^oC^{-1}$)
XNU(I)	- exponential coefficient for swimming speed (s/cm)

E3. Species Type and Sex Classification

MFLG(I), SPBD(I)
(I5,F10.0)

MFLG(I) - flag indicating that this species is a continuation of the last species inputted. Used when a species is divided to separate non-migrating juveniles from migrating adults.

MFLG(I) = 0: species I is a different species than species I-1
MFLG(I) = 1: species I is a continuation of species I-1

SPBD(I) - numbers of julian days after start of calculation to the species birth date

E4. Chemical Uptake Parameters

ASM(I,1), ASM(I, 2), … ASM(I, NCHEM)
(8F10.0)

ASM(I,J) - efficiency at which chemical J is assimilated from food

E5. Growth Pattern

NGBRKS(L)
(I5)

NGBRKS(L) - number of breaks describing annual growth pattern of species I

TIMEG(L,1), WEIGHT(L,1), FLIP(L,1), … TIMEG(L,NGBRKS), WEIGHT(L,NGBRKS), FLIP(L,NGBRKS)

(6F10.0)

TIMEG(L,M) - time of break M in annual growth pattern for age class L (days)

WEIGHT(L,M) - weight of species at time break M (g)

FLIP(L,M) - lipid fraction of species at time break M (g lipid/g wet)

BCF(L,1), BCF(L,2), … BCF(L,NCHEM)

(5F10.0)

BCF(L) - elimination rate multiplier for age class L as described in Group E1

LKOW(L,1), BCF(L,2), … BCF(L,NCHEM)

(5F10.0)

LKOW(L) - partition coefficient of chemical J in species I (L/kg)

Group E7 is repeated NAC(I) times; once for each age class of species I.

Group E is repeated NSP times; once for each age-dependent species.

GROUP F – MIGRATING SPECIES PARAMETERS

F1. Number of Migrating Species

NMIG

(I5)

NMIG - number of migrating species in model

F2. Identification and Migrating Pattern

MIGSN(I)

(I5)

MIGSN(I) - species number of I^{th} migrating species

NBRKS(I), TIMEM(I,J), COMPRT(I,J), … TIMEM(I,NBRKS(I)), COMPRT(I,NBRKS(I))

(I5,5(F10.0,I5),/,5(F10.0,I5))

NBRKS(I) - number of breaks describing the migratory pattern of the I^{th} migratory species

TIMEM(I,J) - time of break J in the migratory pattern of the I^{th} migratory species (days)

COMPRT(I,J) - spatial compartment occupied by the I^{th} migratory species for the time up to TIMEM(I,J)

Group F2 is repeated NMIG times, once for each migrating species. If there are no migrating species, then Group F2 is not to be provided.

GROUP G – SETUP OF SPATIAL COMPARTMENTS

G1. Number of Compartments

NSC

(I5)

NSC - number of spatial compartments included in the model

G2. Compartment Temperature Characteristics

NBRKS2(I)

(I5)

NBRKS2(I) - number of breaks describing the annual temperature and salinity cycles in spatial compartment I

TIMET(I,J), TEMP(I,J) . . . TIMET(I,NBRKS2(I)), TEMP(I,NBRKS2(I))
(8F10.0)

TIMET(I,J) - time of break J in the temperature cycle in compartment I (days)
TEMP(I,J) - temperature at break J in the temperature cycle in compartment I (^{o}C)

G3. Species in Compartment

NSPSI(I)
(I5)

NSPSI(I) - number of species above the plankton level in compartment I

G4. Compartmental Characteristics of the Food Web

G4A. Species Number

SPNO(I,J)
(I5)

SPNO(I,J) - species number of the J^{th} species in compartment I

G4B. Predator-Prey Relationships

NPREY(I,L)
(I5)

NPREY(I,L) - number of prey of species or age class L in compartment I. L is the step number

PREY(I,J,L1), … PREY(I,J,NPREY)
(16I5)

PREY (I,J,L) - step number of the L^{th} prey of step J in compartment I

For example, if a food web consists of plankton, a steady-state invertebrate, and an age dependent fish with 3 age classes the steps are as follows:

	STEP
Invertebrate	1
Fish age 1	2
Fish age 2	3
Fish age 3	4

If fish age 2 preys solely on the invertebrate, then for compartment I PREY (I,3,1) = 1 and PR(I,3,1) = 1.0 (see below). The step numbers for sediment and water column particulates are –1 and –2, respectively.

NTIMEBK(I,L)
(I5)

NTIMEBK(I,L) - number of time breaks describing the feeding preference structure of age class L

TIMEBK(1), PR(L1,I), … PR(NPREY,I) … TIMEBK(NTIMEBK), PR(L1,NTIMEBRK), … PR(NPREY,NTIMEBK)
(8F10.0)

TIMEBK(I) - time of break in feeding preference structure (days)

PR(L,I) - fraction of total consumption constituted by prey L at time break I. The total consumption (i.e. the sum of PR(1,NTIMEBK) through PR(NPREY,NTIMEBK) must equal 1.0. Note that this array does not index the predator.

G4C. Initial Concentrations

CFC(I,L,IC), … (CFC(NCHEM,L,IC)

(8F10.0)

CFC(I,L,IC) - concentration of chemical I in steady-state species or age-class L in compartment IC at the start of the calculation (µg/g wet)

For age-dependent species, subgroups G4B and G4C are repeated for each age class. Groups G3 and G4 and repeated NSPSI(I) times in each compartment I; once for each species in the compartment. Groups G2 through G4 are repeated NSC times; once for each spatial compartment.

GROUP H – PRINTING AND INTEGRATION CONTROL

H1. Printing and Integration Information

DT, TTIME, PRNT, T0, SPRNT

(5F10.0)

DT - time step (days)

TTIME - total run time (days)

PRNT - print interval for outputting concentrations (days)

T0 - julian date at beginning of run (typically 0 days)

SPRNT - time after start of simulation to start outputting concentrations (days)

DEBUG - set to DEBUG in order to print diagnostic files or to NOBUG to avoid printing of diagnostic files.

GROUP I – EXPOSURE CONCENTRATIONS

I1. Number of Values Describing the Temporal Distribution of Concentrations

NCON
(I5)

NCON - number of values of concentrations to be inputted

CWATM(L,I), CPWATM(L,I), CSEDM(L,I), CPSEDM(L,I)
(8X,4F8.0)

CWATM(L,I) - scale factor for water column dissolved concentrations of chemical I in compartment L

CPWATM(L,I) - scale factor for water column particulate concentrations of chemical I in compartment L

CSEDM(L,I) - scale factor for pore water dissolved concentrations of chemical I in compartment L

CPSEDM(L,I) - scale factor for particulate sediment concentrations of chemical I in compartment L

I2. Concentration Profile

TEXP(L,M,I), CWAT(L,M,I,), CPWAT(L,M,I), CSED(L,M,I), CPSED(L,M,I), …
TEXP(L,M,NCON), CWAT(L,M,NCON), CPWAT(L,M,NCON), CSED(L,M,NCON), CPSED(L,M,NCON)

(5F8.0)

TEXP(L,M,I) - time break for chemical I in compartment L (days)

CWAT(L,M,I) - dissolved chemical concentration in the water column in segment L up to time TWAT(L,M,I) (µg/L)

CPWAT(L,M,I,) - adsorbed chemical concentration of chemical I in the water column in segment L up to time (TWAT (L,M,I) (µg/g C)

CSED(L,M,I) - dissolved chemical concentration of chemical I in the sediment in compartment L up to time TWAT (L,M,I) (µg/L)

CPSED(L,M,I) - adsorbed chemical concentration of chemical I in the sediment in compartment L up to time TWAT (L,M,I) (µg/g C)

Group I is repeated for each spatial compartment in sequence and within a compartment for each chemical being modeled.

SECTION 5
OUTPUT FILES

Execution of the bioaccumulation model results in the creation of eight text output files. A description of each output file is detailed below.

FDCHAIN.OUT - contains all echoed input data as well as predicted concentrations for each species

FDCHAINA.OUT - contains a time history of contaminant concentrations and lipid contents for each step modeled (i.e., each steady-state species and each age class of each age-dependent species). Values are provided every PRNT time steps.

Column 1: time since start of simulation (days)

Column 2: spatial compartment

Column 3: biota step number (see Section 1.2)

Column 4: species number (see Section 1.2)

Column 5: species age class (see Section 1.2)

Column 6: chemical

Column 7: wet-weight contaminant concentration (μg/g wet)

Column 8: lipid fraction (g lipid/g wet)

BIOENG1.OUT - contains weight and lipid information for the age-dependent species. Values are provided every PRNT time steps.

Column 1: time since start of simulation (days)

Column 2: biota step number (see Section 1.2)

Column 3: whole body wet weight (g)

Column 4: lipid fraction (g lipid/g wet)

BIOENG2.OUT - contains kinetic and bioenergetic information for the age-dependent species. Values are provided every PRNT time steps.

Column 1: time since start of simulation (days)

Column 2: spatial compartment

Column 3: biota step number (see Section 1.2)

Column 4: species number (see Section 1.2)

Column 5: species age class (see Section 1.2)

Column 6: weight (g)

Column 7: growth rate (g wet/g wet-day)

Column 8: lipid fraction (g lipid/g wet)

Column 9: energy content (kJ/g wet)

Column 10: growth rate (kJ/g wet-day)

Column 11: respiration rate – intermediate calculation (kJ/g wet-day)

Column 12: respiration rate (kJ/g wet-day)

Column 13: food consumption rate (kJ/g wet-day)

Column 14: food consumption rate. When consumption rate is computed to be less than zero, it is set equal to zero. In this case, Column 14 provides the originally computed rate. Otherwise, Column 14 is set equal to zero. (kJ/g wet-day)

DOSE.OUT - contains summary of contaminant uptake and loss rate terms for all steady-state and age-depenedent species. Values are provided every PRNT time steps.

Column 1: time since start of simulation (days)
Column 2: spatial compartment
Column 3: biota step number (see Section 1.2)
Column 4: species number (see Section 1.2)
Column 5: species age class (see Section 1.2)
Column 6: chemical
Column 7: uptake rate from water (L/g wet-day)
Column 8: chemical uptake rate from food (µg/g wet-day)
Column 9: sum of chemical loss terms (excretion + growth) (day^{-1})

EXPOSE.OUT- Not used in current version of model.

LOSS.OUT - contains contaminant loss rate terms for age-depenedent species. Values are provided every PRNT time steps.

Column 1: time since start of simulation (days)
Column 2: spatial compartment
Column 3: biota step number (see Section 1.2)
Column 4: species number (see Section 1.2)
Column 5: species age class (see Section 1.2)
Column 6: chemical
Column 7: chemical elimination rate (day^{-1})
Column 8: chemical uptake rate from food (µg/g wet-day)

Column 9: growth rate (g wet/g wet-day)

PREY.OUT - contains food web structure and dietary preference information for all steady-state and age-depenedent species. Values are provided every PRNT time steps.

Column 1: time since start of simulation (days)
Column 2: spatial compartment
Column 3: chemical
Column 4: biota step number (see Section 1.2)
Column 5: species number (see Section 1.2)
Column 6: species age class (see Section 1.2)
Column 7: index number for species in compartment
Column 8: prey step number
Column 9: fraction of total energy consumed for each prey species
Column 10: contaminant concentration of prey ÷ energy density of prey (μg/kJ)

TEST.OUT - contains debugging information. Not used in current version of model.

WARNINGS.OUT - contains warnings concerning model parameter values